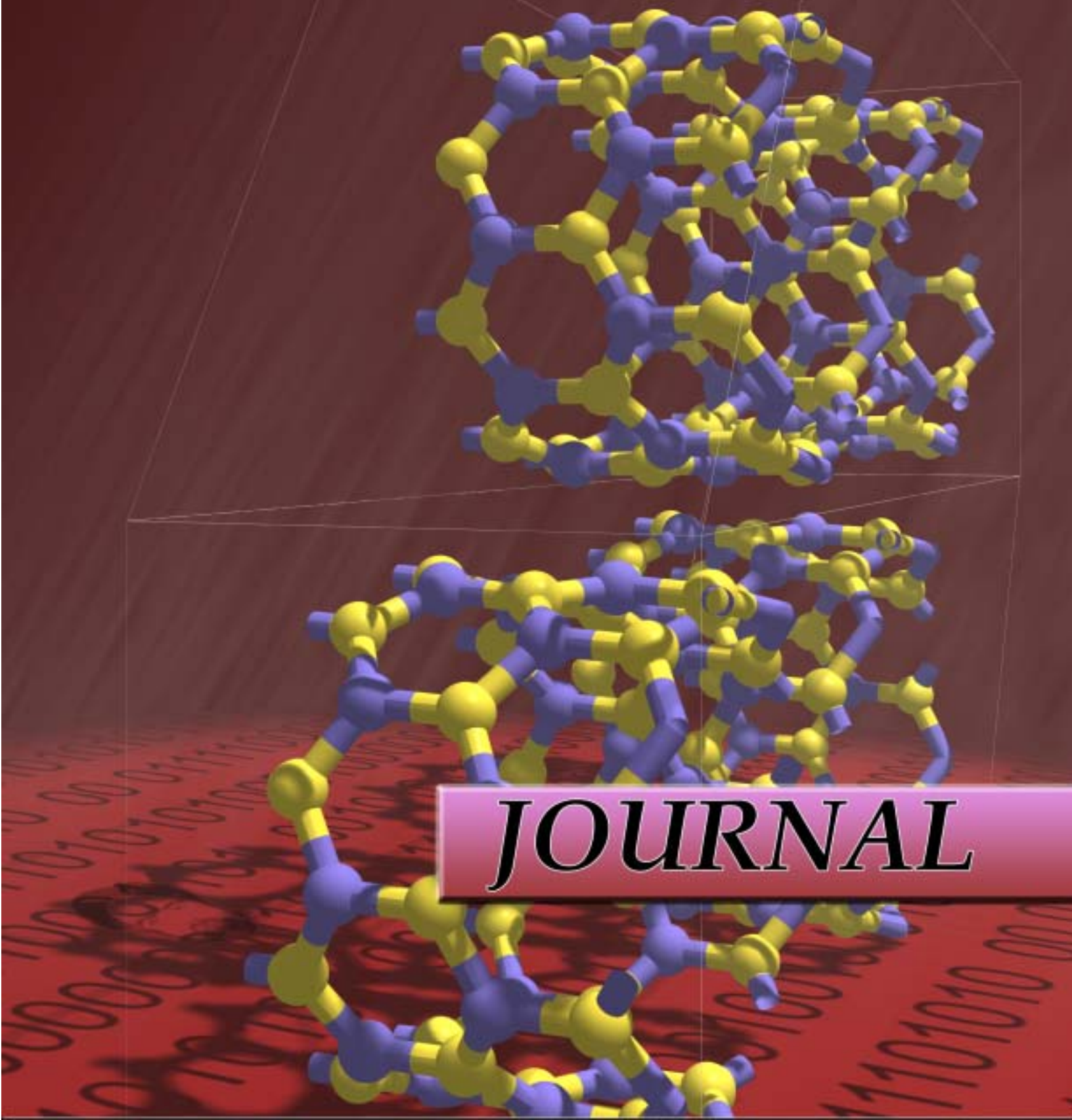
FALL 2002

ASC MSRC

AERONAUTICAL SYSTEMS CENTER

MAJOR SHARED RESOURCE CENTER



JOURNAL

The Aeronautical Systems Center (ASC) Major Shared Resource Center (MSRC), is a computational science facility supporting Department of Defense (DoD) research, development, and test and evaluation communities with high performance computing and visualization resources. It was created as part of the DoD's High Performance Computing Modernization Program (HPCMP). The ASC MSRC High Performance Computing Center is located on Wright-Patterson Air Force Base (WPAFB) and is one of four DoD MSRC sites. Computer Sciences Corporation (CSC) Defense Group is the prime contractor and system integrator at the ASC MSRC.

ASC MSRC Journal

Fall 2002 Volume 6.2

The Director's Desk

Steve Wourms

Here we go, my second installment in this most august journal! I have lost the "interim" part of my title, and am now about as permanent as one gets in this position at the ASC.

These are certainly exciting days at the ASC MSRC. What with contract changes looming, anticipation of TI-03, and the DoD divesting itself of this HPC Modernization Program. We are operating in interesting times.

I invite you to check out the slate of articles in this journal. Lisa Burns describes our approach to establishing a disaster recovery capability for our center's data holdings. Jeff Graham provides a progress report on TI-03. Software updates are announced by the Computational Technology Center staff. Network upgrades are covered by Ralph McEldowney.

While all these management and operational issues swirl about, our Center's users continue in their clamoring for more and more capacity. And of course, there are articles on our users' activities, both from DoD researchers and by our latest crop of summer interns.

Finally, we are bidding adieu to a long time fixture at our MSRC. Mike Moore will have retired from government service by the time this journal is published. Mike's the guy most notorious for lurking around our booths at the myriad of conference appearances by the ASC MSRC. Always quick to engage a passer-by on the conference floor, he was renowned for his itchy shutter button finger, looking to capture a moment in digital permanence. We will certainly miss Mike and all of his contributions, and wish him Godspeed as he joins his family in Indiana to teach Algebra at a local community college.

I signed off my last journal installment citing those immortal words of Jeff Graham in describing today's environment, "It was the best of times, it was the worst of times."

Let's work together for the sake of the warfighter and have some fun in the process!

Table of Contents

The New ASC MSRC Disaster Recovery System

by Lisa Burns

The formation of the Mass Storage Archive System (MSAS) Working Group (WG) by the High Performance Computing Modernization Program (HPCMP) in December 1998 was critical to address the phenomenal data growth rates experienced by many of the HPCMP sites. In November 1996 the ASC MSRC started with 50 Gigabytes (GB) of total tape archive data and today has more than 140 Terabytes (TB). Monthly growth rates average 5 TB/month and this is after a 50% deletion/clean-up rate by the users. As the amount of user data continues to grow, so does the importance of protecting this user data.

The MSAS-WG's members agreed upon a basic MSAS architecture built upon some common functional hardware and software components. Key concepts of the MSAS architecture included high availability, significant scalability, high performance, flexibility, and security. With the ever-increasing data growth, these new mass storage systems needed to be able to protect the users' data, while still allowing the users the capability to store and retrieve their data as quickly as possible. A longer-term MSAS-WG objective was that each site's MSAS architecture could be easily expanded into a geographically distributed disaster recovery (DR) solution, with as much reuse of software and hardware as possible.

Current ASC MSRC MSAS System Overview

In keeping with the MSAS-WG's objectives, the ASC MSRC embarked on a multi-year plan beginning with a total MSAS overhaul in 1999. This overhaul implemented a new highly available and high-performing mass storage system, introduced the beginnings of a Storage Area Network (SAN) infrastructure, and upgraded the network to OC-12 Asynchronous Transfer Mode (ATM) and Gigabit Ethernet. The 1999 changes replaced the old storage server and single library control workstation with two clustered Sun Enterprise 10000 servers and two clustered library control workstations; added an additional library storage silo; replaced older tape drives with 12 new StorageTek 9840 SCSI tape drives; added additional tape media; and replaced the older 300 GB of storage disks with 1.8 TB of newer disks. Each of the two mass storage servers and two library control workstations were clustered together using Veritas Cluster Server (VCS) software. Using standard and newly developed VCS agents, fast and robust application and server fail-over capabilities were attained without impacting the user.

Also in 1999, new Hierarchical Storage Management (HSM) and high performance file system software, known as Storage Archive Manager-Quick File System (SAM-QFS), was installed. SAM-QFS efficiently controls data in the ASC MSRC's archive by combining a high performance file system and volume management with integrated storage and archive management features. By automatically and transparently copying files from the on-line disk to the tape storage libraries, SAM-QFS gives the appearance of an infinite disk to users.

In late 2000, the Redundant Array of Inexpensive Disks (RAID) was upgraded to more than 3 TB. A Fiber Channel (FC) switch was installed to provide the ASC MSRC MSAS with a more robust SAN back-end architecture that would allow for future improvements. In October 2001, six newer and higher capacity StorageTek 9940 FC tape drives were added, in addition to the existing 9840 SCSI tape drives being upgraded to fiber. Half of the 18 tape drives were connected to the SAN by an FC switch, while the other half were connected by a second FC switch. A third FC switch, used to connect the RAID and the E10000 servers, enhanced the overall system availability and allowed for an even faster fail-over capability since the fiber tape drives no longer had to be managed during an actual fail-over. In late 2002, MSAS performance will be further enhanced when additional system boards, CPUs, memory, and network adapters are added to each of the Sun E10000 servers.

The New ASC MSRC Remote DR System

The ASC MSRC and the Space and Naval Warfare Systems Center – San Diego (SSC-SD) have entered into a partnership to provide mutual disaster recovery capabilities. Each site is providing the necessary facilities (e.g., space, power, and cooling) to support the respective systems. The basic idea is to share common resources, where it is most appropriate. The common resources include the storage silos, and their respective auxiliary equipment such as the library management units and library control units, and the Automated Cartridge System Library Software (ACSLS) tape robotics control software and workstations. Each site will have dedicated tape drives with their own dedicated pools of tape media located within these shared libraries.

The respective DR systems will become operational in a phased approach. The primary goal of this new system

is to allow a third copy of user data and system backup data to be stored automatically, transparently, and in near real-time to SSC-SD so that, in the event of a major catastrophe, MSRC data will not be permanently lost. A secondary goal for the ASC MSRC is to be able to recover data on a smaller scale (single file or subsets of files such as a file system) and on a more ad hoc basis, in the event of a smaller-scale error, such as a human error.

The ASC MSRC will use the Defense Research and Engineering Network (DREN) to transfer data between the two sites. Initially, an ATM Permanent Virtual Circuit (PVC) will be created over DREN. An IP-based solution will be explored in the future. In addition, the data will be encrypted during transit using a FIPS 140-1 compliant algorithm.

The new DR system installed at SSC-SD includes a rack-mounted system containing an ACSLS server (library management server), a SAM-QFS HSM server, 1 TB user capacity RAID, one Brocade 3800 FC switch, and a network router. Additionally, the ASC MSRC will provide a stand-alone StorageTek 9310 Powderhorn silo six StorageTek 9940a tape drives, and a large number of StorageTek tape media cartridges.

The functional components of the existing ASC MSRC MSAS system remain essentially the same however, minor hardware modifications to the mass storage and network infrastructure systems are required to support the new DR requirements. The current FC HSM RAID system will be replaced with a newer slightly higher capacity and higher performing disk cache system. The current six 9940a tape drives (60 GB and 10 MB/sec) will be replaced with six 9940b tape drives (200 GB and 30 MB/sec). The six 9940a tape drives will be re-utilized in the silo at SSC-SD.

In the future, SSC-SD will provide their own Sun server (with disks), a fibre channel switch, and a router to connect their Sun server to the DREN connection at the ASC MSRC. An Ethernet connection will allow the SSC-SD system to connect into the ASC MSRC ACSLS systems and to access the SSC-SD dedicated tape drives.

A new version of the SAM-QFS software that has been used at the ASC MSRC will play a critical role in this new DR system. The current SAM-QFS product supports local disk and local tape as a destination for archive copies. SAM-QFS 4.0 provides all of the functionality as provided in the current release of SAM-QFS as well as providing the additional capability to archive and stage to either a remote tape archive and/or to a two- tier remote SAM-QFS disk cache. This software allows for standard SAM-FS releasing of the local disk cache file after an archive copy exists on the remote server. The disk cache used for disk archiving may actually be another local file system or a remote SAM-FS file system. The files are automatically and transparently copied to the alternate disk cache according to the archive set rules. In 4.0, the remote disk cache is treated simply as another form of archiving media and the files being written to the remote disks are the actual SAM tar files.

The mass storage upgrades performed over the past several years have provided the users with a more flexible, highly-reliable, and high performing system that should continue to scale well into the future with the current data growth projections. The new remote DR system, planned for implementation in late 2002, is a natural extension to the existing mass storage system and will provide the users with another level of much-needed data protection.

Technology Insertion 03 – Progress Report

by Jeff Graham

As we approach the end of the calendar year, things are heating up at the four MSRCs. The Collective Acquisition Team (CAT) – comprised of the directors and other participants at the four centers and managed by John Blair from the HPCMO – gears up for the next set of upgrades at the centers. The CAT has reviewed user requirements and other acquisition factors in order to develop a Request for Quotes (RFQ) for potential hardware upgrades for the centers. The process, initiated by the HPCMO two years ago, is known as the Technology Insertion (TI) process. Since the timeframe for the arrival of the new equipment is in the Spring of FY03, this year's process is referred to as TI-03.

The long process started soon after last year's process (TI-02) was completed. The results of TI-02 included major upgrades at both the Army Research Laboratory (ARL) and the Naval Oceanographic Office (NAVO) (specifically a significant amount of the latest HPC technology from IBM known as the Regatta) and infrastructure upgrades (software, Mass Storage, etc.) at both ERDC and ASC. TI-03 targets major upgrades at ERDC and ASC – so the staff at the ASC MSRC are excited about the realization of a significant bump in HPC resources for our user community. ASC MSRC users can look forward to modernized and usable resources on the horizon to improve throughput and turnaround. The last major upgrade, which was the result of TI-01, consisted of the Compaq ES45 being installed in the winter of 2001.

The CAT is on schedule to release the final RFQ in late October, receive final solution set responses in late November, and make a recommendation to the Director of the HPCMO in mid-December. Evaluation teams will consider cost, performance (through benchmark analysis), confidence and usability in making decisions that will most effectively and aggressively meet user requirements. The plan is to have the new hardware on the floor by late March and have the systems available for the user community no later than late June.

Although anticipation runs high, the CAT is confident that users will be happy with the results of the TI-03 process. Given two years of prior experience, the process has been refined through continuous process improvement techniques, and should result in a major step forward for the program.

Software Updates

by Casey Doty and Jason Stare

The ASC MSRC recently added two software packages to the SciVis suite and an application of interest to our Computational Fluid Dynamics (CFD) community.

Both Vis5D and Grid Analysis and Display System (GrADS) aid users in pre- and post-processing of computational weather data. Vis5D is a system for interactive visualization of large 5-D gridded data sets such as those produced by numerical weather models. Formerly developed at the Space Science and Engineering Center, Vis5D has recently been open-sourced at *www.sourceforge.net*, and renamed Vis5D+. Open-sourcing the program has allowed development to continue and extra features, such as OpenGL and ImmersaDesk/CAVE support to be added. Plans to add Vis5D+ to the ASC MSRC ImmersaDesk demo are currently underway.

GrADS is an interactive desktop tool that is used for easy access, manipulation, and visualization of earth science data. The format of the data may be either binary, GRIB, NetCDF, or HDF-SD (Scientific Data Sets). GrADS has been implemented worldwide on a variety of commonly used operating systems and is freely distributed over the Internet. While GrADS currently does not support ImmersaDesk or CAVE libraries, it does provide users specializing in earth science a great tool for visualizing and manipulating their data.

The addition of Vis5D and GrADS to the ASC MSRC's already expansive arsenal of visualization software, provides users another method to use when visualizing and manipulating weather and geographical data.

Cobalt, a cell-centered, finite volume CFD code from Cobalt Solutions, provides advanced CFD analysis capability for a variety of applications. Like the CHSSI version of Cobalt, this *commercial* Cobalt supports several additional features such as rigid-body motion, expanded Detached Eddy-Simulation (DES) for treatment of massively separated flows and equilibrium air physics.

Cobalt supports common boundary conditions such as solid-walls, farfield, and rotor/prop conditions to name a few. In addition, the user can easily add a Fortran 90 module to create custom boundary conditions and integrate them into the code.

The application scales very well on a variety of distributed memory parallel architectures that allow researchers to solve extremely large problems very quickly. Cobalt can accept any polyhedral elements in a grid including hybrid grids. Already in place at the ASC MSRC are Gridgen and ICEM, grid generators that support Cobalt grid formats.

Cobalt contains state-of-the-art turbulence models including Spalart-Allmaras, Menter's SST, Wilcox's 1998 k-w, and DES for Spalart and Menter's Models.

Cobalt outputs directly to several leading post-processing formats, eliminating the need for tedious converters. The output files are in the post-processor's native format, resulting in less time and less memory, when reading in results. Time-dependent files can be written to allow for easy visualization of unsteady data. In addition to Cobalt (native format), Ensight, Fieldview and Tecplot are post-processing formats available at the ASC MSRC.

For more information on this application go to *www.cobaltcfd.com.*

Network Upgrades Keep MSRC in the Fast Lane

by Ralph McEldowney

The ASC MSRC recently completed a major network upgrade, which significantly increased the bandwidth between the high-performance computers and positions the MSRC for future Defense Research and Engineering Network (DREN) upgrades. These upgrades were completed as part of the MSRC's TI-02 enhancements.

The MSRC operates multiple highly robust and reliable high-performance networks. These local area networks connect the high-performance computers, file servers, visualization servers, and support servers with DREN, providing access to users located around the country. With the TI-02 upgrades, there are now two high-speed backbones and several administrative networks.

The primary high-speed backbone is the new Gigabit Ethernet jumbo frame network. This network operates at 1000 megabits per second, and supports Ethernet packet sizes up to 9000 bytes. This is a significant increase over the standard Ethernet frame size of 1500 bytes. To implement this network, the MSRC selected Foundry Networks' BigIron 15000 switch/router with third generation JetCore ASICs. This network supports up to 120 Gigabit Ethernet connections, and is used for NFS traffic between the compute and file servers.

The second high-speed backbone is an Asynchronous Transfer Mode (ATM) OC-12 network. This network operates at 622 megabits per second, and supports both the Classical IP (CLIP) protocol with frames sizes of 9180 bytes, and the LAN Emulation (LANE) protocol with frames sizes of 1500 bytes. The ATM switch supporting this network is a Marconi ASX-4000 with 60 OC-12 ports and 16 OC-3 ports (155 megabit per second). The router supporting the CLIP network is a Cisco 12008 with dual OC-12 interfaces, while the router supporting the LANE network is a Cisco 7513 also with dual OC-12 interfaces. TI-02

enhancements included the addition of 16 OC-12 ports for the ASX-4000 and an upgrade for the LANE router from OC-3 to OC-12. The ATM network is used for remote user access and local system backups.

The administrative networks are based on Ethernet (10 megabits per second), Fast Ethernet (100 megabits per second), and Gigabit Ethernet (1000 megabits per second), all using 1500 byte standard frames. These networks were also enhanced in TI-02. A Foundry Networks' BigIron 15000 switch/router replaced a smaller switch, which significantly increased the number of available ports. The new switch supports up to 144 Ethernet/Fast Ethernet connections and 72 Gigabit Ethernet connections. This network is used for the administrative interface on compute and file servers, and for the primary interface on support servers.

Other administrative networks support the MSRC classroom and staff workstations located throughout the MSRC facility. These networks are implemented with six existing Foundry Networks' FastIron2 switches, each containing 72 Ethernet/Fast Ethernet ports and dual Gigabit Ethernet uplink ports.

In addition to all the enhancements in the local area networks, the MSRC also significantly enhanced its DREN connection capabilities by acquiring a new border router. The previous border router was more than five years old, and was no longer capable of meeting the bandwidth, throughput, and port density requirements of the MSRC. For the new border router, the MSRC selected Juniper Networks' M20 Internet Router. The Juniper M20 provides more than 20 gigabits per second throughput, fully redundant capabilities including route processors and system boards, and greatly increased port densities. For example, the M20 supports up to 16 Gigabit Ethernet ports, 16 ATM OC-12 ports, 16 OC-12 Packet Over SONET (POS) ports, four OC-48 (2.5 gigabits per second) POS ports, or various combinations of these interfaces. This router not only significantly improves the current border router capabilities, but also positions the MSRC for future DREN OC-48 connectivity requirements.


Foundry BigIron 15000


Juniper M20

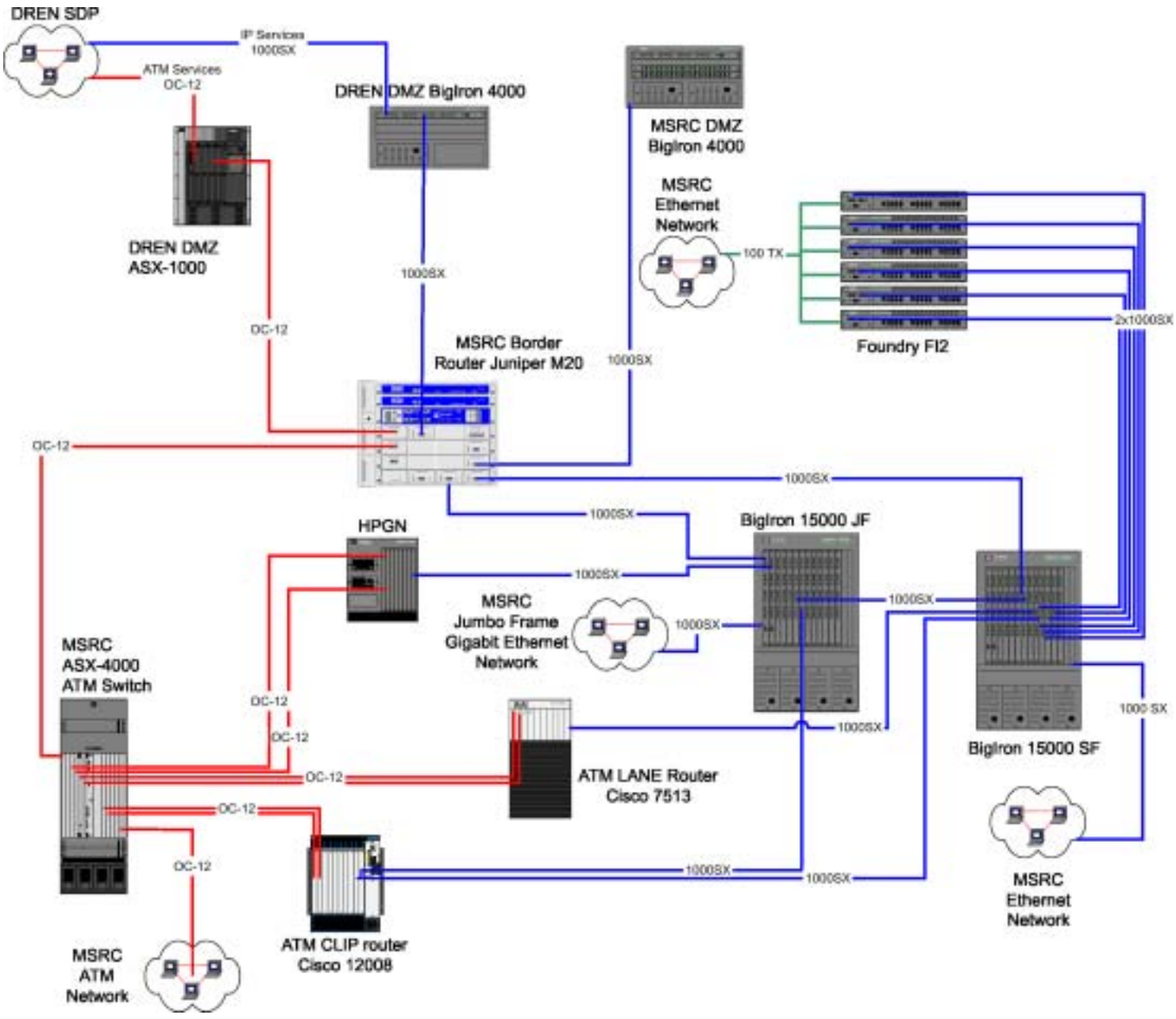

Cisco 12008


Marconi ASX-4000

The recently completed TI-02 network upgrades continue to keep the ASC MSRC at the forefront of the high-performance networking community. Hopefully, these enhancements to the border router, NFS environment, and administrative networks will help the MSRC support staff and all ASC MSRC users to be more efficient and productive.

For additional information or to report problems with the MSRC network or DREN connectivity, please contact the MSRC Service Center at 1-888-MSRC-ASC.

ASC MSRC Target TI-02 Configuration



Year 1 Contract Review

by Jeff Graham

The government oversight team for the Programming Environment and Training (PET) program conducted the first contract review since awarding contracts for each of the four components in June of 2001. Components 1, 2, and 3 were awarded to the MOS Consortium led by Mississippi State University and Ohio Supercomputer Center, while component 4 was awarded to High Performance Technologies, Inc (HPTi). The Engineer Research and Development Center (ERDC) in Vicksburg, Mississippi served as the host for the event held May 13-17.

The PET program enables the DoD HPC user community to effectively leverage HPCMP resources; thereby extending the range of technical problems solved on HPC systems to more positively impact weapons system developments. PET is enhancing the total capability and productivity of the program's user community through training, collaboration, tool development, support for software development, technology tracking, technology transfer, and outreach.

In the area of overall program management the HPCMP PET Program Manager, Dr. Leslie Perkins, acts as chairperson of a board of directors composed of the four technical advisors (TAs), one located at each MSRC. The TAs for each component are:

Component 1 – Eleanor Schroeder, Naval Oceanographic Office (NAVO)
- Climate/Weather/Ocean Modeling (CWO)
- Environmental Quality Modeling (EQM)
- Computational Environment (CE)

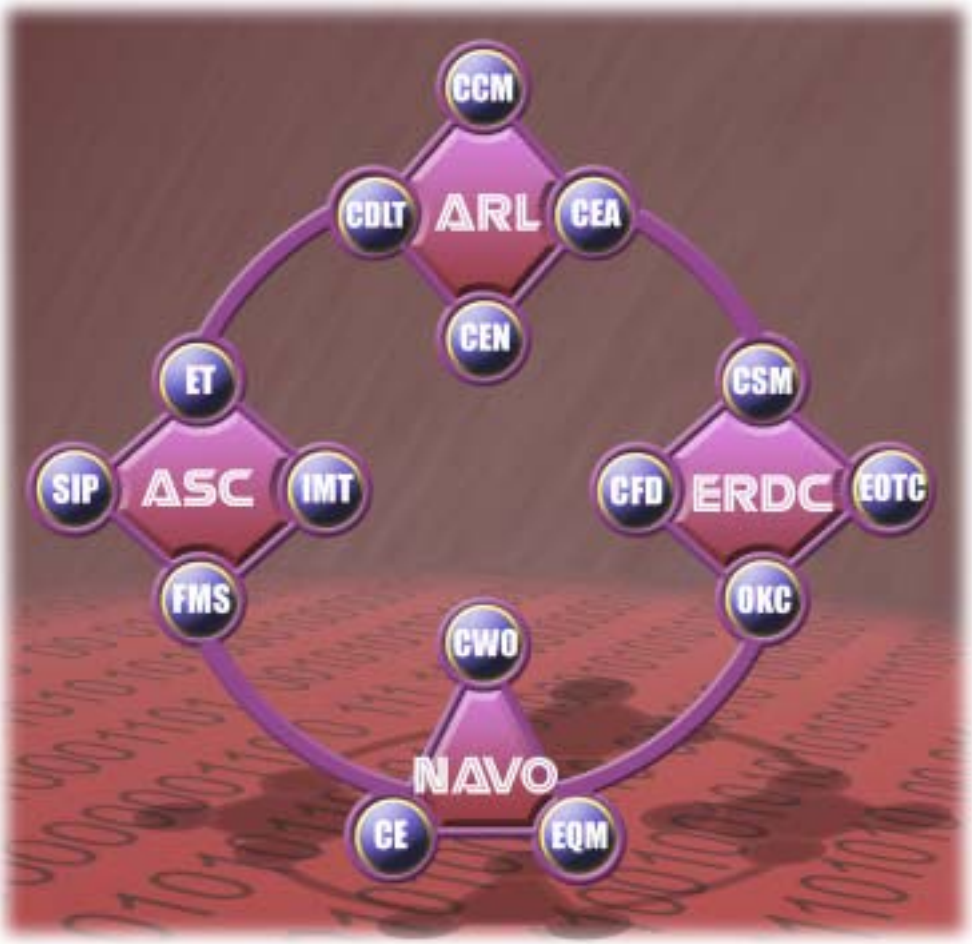
Component 2 – Brian Schafer, Aeronautical Systems Center (ASC)
- Signal Image Processing (SIP)
- Forces Modeling and Simulation (FMS)
- Integrated Modeling and Testing (IMT)
- Enabling Technologies (ET)

Component 3 – Robert Athow, Engineer Research and Development Center (ERDC)
- Computational Fluid Dynamics (CFD)
- Computational Structural Mechanics (CSM)
- Online Knowledge Center (OKC)
- Education Outreach & Training Coordination (EOTC)

Component 4 – Andrew Mark, Army Research Laboratory (ARL)
- Computational Chemistry & Materials Science (CCM)
- Computational Electromagnetics & Acoustics (CEA)
- Computational Electronics & Nanoelectronics (CEN)
- Collaborative & Distance Learning Technologies (CDLT)

This team, along with HPCMP Director Cray Henry and invited Computational Technology Area (CTA) leaders, Jeff Holland (EQM), Robert Meakin (CFD), and William Burnett (CWO), evaluated the performance of the contractors in the first year. Reviews were solicited in overall program management from each contractor, overall component activities from the Component Point Of Contacts (CPOCs), and in each Functional Area (FA) from the corresponding FA Point of Contact (FAPOC). Templates for the presentations and guidelines for the formal process were developed by the review team and communicated to the contractor teams in order to provide order to the proceedings. Each CPOC and FAPOC were given an equal amount of time to brief the team. Following a short break, a structured question and answer period was held to address concerns from the review team.

The MOS team presented activities in their areas of responsibility Monday through Thursday, and HPTi presented on Friday. Although it was a grueling experience for members of the review team, it was an informative and enlightening overview of contractual aspects of the performance over the first year of the contracts. At the end of each day, the reviewers met to develop an overall assessment of activities in the areas reviewed. Preliminary feedback was presented to the contractor teams at the end of their review. Within two weeks of the overview, the review team provided the contractors with a formal assessment document. The assessment included a rating for each area of review (ranging from unacceptable, marginal, acceptable, and excellent), a summary of strengths and weaknesses, and a set of recommendations as well as required actions. Ratings varied across the FAs and the contractors agreed to take remedial actions in areas of poor performance.



Special thanks should be relayed to the ERDC team that hosted the review. The accommodations and facilities were top notch! The PET government oversight team was pleased to accomplish this important milestone for the program, and looks forward to the technical review being planned for early in 2003.

PET Summer Interns 2002

by Nicholas Voiles

The 2002 PET summer interns traveled from far and wide to participate in another high performance computing filled summer. Various colleges and universities around the country were represented this summer. Schools represented included the Worchester Polytechnic Institute, the Rose-Hullman Institute of Technology, Massachusetts Institute of Technology (MIT), and Wright State University (WSU). Experiences like these give students the opportunity to take what they have learned in the classroom, and put it to the test in a real world work environment. Additionally, the MSRC staff gains valuable help for the summer, and the interns get first hand experience working on real DoD projects. Tyler Ryan, from the Rose-Hullman Institute of Technology had this to say when asked about the program, "My summer projects have helped to familiarize me with being an engineer and a researcher in general. I felt as if I made a difference here helping solve real world problems."

For the first time in the history of the PET summer intern program, the PET contractors coordinated the program across all four MSRCs. The goal was to work with the four centers to manage a program-wide intern program, while maintaining the uniqueness of each centers prospective intern program. "Even though the PET contractors got a late start in organizing the program it was still a success. Sue Brown from the Ohio Supercomputer Center (OSC) led the effort to plan and implement the program," commented Jeff Graham, former ASC MSRC PET Government Lead. Some of the other key players in the program were Bill Zilliox (CSC), Sharron Madero (OSC), and Mason Colbert (OSC). "This new program also gave us a chance to see what was going on at the other MSRCs around the country," mentioned Graham.

Danny Vereen Jr. made the journey from Florida A&M University in Tallahassee, Florida. A junior, dual Computer Engineering and Electrical Engineering major, Vereen worked with Mason Colbert and Dr. John Nehrbass, Signal Image Processing on-site lead, throughout the summer. The first part of the summer Vereen focused on developing a JavaScript function to be inserted into a registration form with the ability to detect and notify the user of errors, and also remember specific user information for future registration. Vereen stated, "I was somewhat familiar with the HTML language before I came, but I improved my skills in both HTML and JavaScript while I was here for the summer." The second half of the summer Vereen focused on a 3-D graphics accelerator with fellow intern Greg Grieco and Dr. Nehrbass. Grieco is a junior Electrical Engineering major at the Ohio State University. He heard about the PET summer intern program from his teacher, Professor Stanley Ahalt who has worked with Dr. Nehrbass in the past.

Jonathan Moussa and Jacob Gagnon worked together as a team throughout their summer here at the MSRC. Moussa focused on the Schrodinger-Poisson Self-Consistency in Semiconductor Heterostructures. Dr. Paul Sotirelis, Computational Electronics and Nanoelectronics (CEN) on-site lead, was his mentor. Moussa is a graduate student at the Worchester Polytechnic Institute in Massachusetts. He was also an intern here in the summer of 2000 and is looking forward to completing his Masters degree at Berkeley next year. Jacob Gagnon is a graduate student as well, and came to us from the MIT. His summer project involved TeraHertz emitter modeling and his mentor was also Dr. Sotirelis. His research relates to TeraHertz lasers, which could have a major role in the future for use with various medical and communications applications, and even play a part in airport security environments. (*See related article page 19*.)

Travis Franck is a senior majoring in Mechanical Engineering from Case Western Reserve University in northern Ohio. He came back for a second year of learning and research at the MSRC. He kept in touch throughout the 2002 school year with Dr. Jean Blaudeau, Computational Chemistry and Materials Science (CCM) on-site lead. Dr. Blaudeau was Franck's mentor last summer and worked with him this year as well. Franck built on his project from last year and performed energy calculations on C_{122} complexes. He also calculated the lowest energy bridge and showed the C_{122} complexes visually. In describing his experience here Franck said, "This summer I've been working on a project that will actually help out the DoD in the future. The ASC MSRC needed my help to complete these tasks and has shown me what it's like to be part of a real project."

Rebecca Busch is another intern who returned to the ASC MSRC. This is the third year in a row that she has visited WPAFB to complete another summer full of hard work. She kept in touch with the staff at the MSRC this past year as she concluded her junior year at Ohio Northern

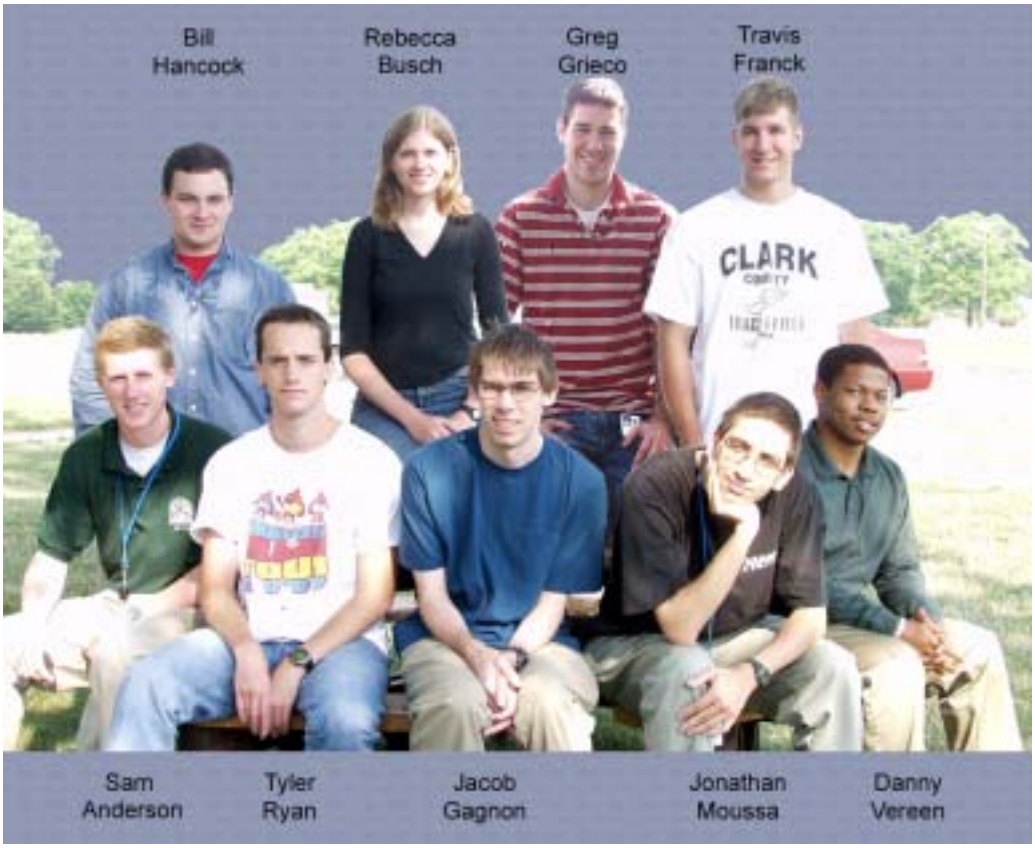
University. “During my third summer as an intern at the ASC MSRC, I have had the opportunity to hone my Java skills on a software program known as Encrypted Web Information Transfer (EWit). When I began work this summer I was given a release version of EWit and the task of discovering existing bugs in the program,” remarked Busch. Her mentor for the summer was Dr. Nehrbass. (*See related article page 17*.)

Samuel Anderson recently graduated from WSU, and has chosen to continue working on his Master’s degree at WSU as well. He focused on Mechanical Engineering, and his mentor for the summer was Dr. Hugh Thornburg, Computational Fluid Dynamics (CFD) on-site lead. In describing his summer here, Anderson had this to say, “I have met many interesting people and have done a lot of networking throughout my time here. I am currently inquiring about a co-op which would allow me to continue working here as I complete my Master’s degree at WSU. Working for the government seems to be very rewarding, and I would love to work here full-time once I complete my studies.” Anderson’s past work experiences include internships at both Delphi and Dayton Power and Light. His work this summer involved utilizing CFD to study and research the various effects of stress on aircraft wings. These types of studies will help engineers build safer and more efficient planes in the future.

Studies of platinum-containing oligomers filled William Hancock’s head from June through August. Making the trip from Birmingham Southern College, Hancock knew he would be faced with a tough, yet exciting, summer full of physics. Dr. Blaudeau mentored him throughout the summer, and gave him valuable information about the project. When describing his summer work Hancock said, “My objectives were to develop novel nonlinear dyes for photonic applications. We were interested in mapping out the photophysical properties of a series of platinum poly-yne oligomers and polymers.” This type of research definitely followed along with his major and gave him an idea of what the DoD is currently focusing on. When asked about the hardest things he came across this summer Hancock said, “Getting used to a secured, government controlled research environment took some getting used to, but it was definitely a very valuable experience for me.”

A junior Mechanical Engineering and Computer Engineering dual major, Tyler Ryan was mentored by Dr. Thornburg although he also worked along with Dr. Mohammed Mawid (ASC/PRTC). His summer endeavors included designing a graphical user interface, and designing a program to test the feasibility of grid subdivision for the solution adaptive grid strategies. Ryan had these positive words to say about the program, “It has been great working at one of the DoD’s high performance computing centers. This summer intern program has been very worthwhile, and now I have a better idea of how the research community works.”

Students who are interested in pursuing a career-broadening internship will have the chance again in the summer of 2003. To apply for the HPC Summer Intern Program, please contact Sharron Madero at *sharron.madero@wpafb.af.mil* or Bill Zilliox at *william.zilliox@wpafb.af.mil*.



Beyond the Box

by Chuck Abruzzino

Some of the best high performance visualizations go unnoticed, never making it beyond a single image in a PowerPoint presentation or Viewgraph. The need for marketing research beyond a conference of his peers may seem unnecessary to a researcher or scientist.

At some point the research will have to compete in arenas with other projects. How well the research communicates its importance within the DoD community may fall short of expectations. Understanding the importance of an effective presentation is the first step. The ability or knowledge of resources available to create the most effective presentation requires assistance.

Supporting the ASC MSRC community are services beyond the box, so to speak. As a part of the Customer Assistance Center these services include a large format high-resolution printer, a 40" wide laminator, a CD duplicator/printer, digital photography and videography, computer animation, and a Video Preparation Facility.

Avid Express, a non-linear video and audio editing system, is the core software/hardware in the Video Preparation Facility. Avid offers a full array of digital video effects as well as character-generated text. Narration, music, and sound bytes can be included to improve the effectiveness of the production. PowerPoint presentations can be enhanced with narration and music to create an audiovisual presentation. Still images, such as JPEG, RGB, and many other image formats are easily imported into the Avid for use in the final edited product.

Movie files, such as AVI, SGI, MPEG, and QuickTime can also be utilized. In order for movie files to be imported for use in editing or to transfer movie files to videotape, they must first be readable by others. A format of 720 x 486 pixels is the optimal size and resolution to use for editing. The final edited production can be transferred to videotape (formats include Digital Betacam, Betacam SP, DVCPro, 3/4" U-Matic SP, Hi-8, S-VHS, and VHS) or can be saved as any of the movie file formats mentioned earlier.

Supporting this technology is a staff that understands the marketing needs of the researcher. These professionals stand ready to think out of the box to enhance your next presentation or create material that gets your research noticed and remembered.

Products produced by these professional services are broadcast quality videos on tape, CD or DVD, and authored interactive multimedia CDs.

For a consultation appointment contact the ASC MSRC Customer Service Center, at *msrchelp@asc.hpc.mil*.

FY03 Challenge Projects

The High Performance Computing Modernization Office (HPCMO) has designated approximately 25% of total High Performance Computing Modernization Program (HPCMP) computational resources to be allocated for large, computationally intensive projects. These projects, referred to as DoD Challenge Projects, require the use of DoD HPCMP shared resource center systems.

Prior to the start of each fiscal year, the HPCMO allocates computational time to these projects, based on proposals submitted by the service agencies. In June, the HPCMO announced FY03 challenge projects. Eleven of the thirty-nine projects will run at the ASC MSRC.

Returning from FY02

- New Materials Design - Air Force
- Time-Accurate Computational Simulations of Ship Airwake for Dynamic Interface (DI), Simulation and Design Applications - Navy
- Unsteady RANS Simulation for Surface Ship Maneuvering and Seakeeping - Navy
- High Fidelity Analysis of UAVs Using Nonlinear Fluid/Structure Simulation - Air Force
- Multiscale Simulations of High energy Density Materials - Air Force
- Large-Eddy Simulation of Tip-Clearance Flow in a Stator-Rotor Combination - Navy
- Evaluation and Retrofit for Blast Protection in Urban Terrain - Army

New in FY03

- Numerical Modeling of Turbulent Wakes for Naval Applications - Navy
- Three-Dimensional CFD Modeling of the Chemical Oxygen-Iodine Laser II - Air Force
- Multidisciplinary Applications of Detached-Eddy Simulations of Separated Flows at High Reynolds Numbers - Air Force
- Defense Against Chemical Warfare Agents (CWAs) and Toxic Industrial Chemicals (TICs): Filtration, Prophylaxis and Therapeutics - Army

A salute to Mike Moore, for many

OUTSTANDING CIVILIAN CAREER SERVICE AWARD

Mr. Michael S. Moore is recommended for the Outstanding Civilian Service Award in recognition of his distinguished service as a civil service employee for both the United States Army and Air Force.

Maria Zimmer:
Mike Moore is one, if not the, nicest person I've ever worked with. His work is always thorough and professional. He is very personable and always considerate of others. When he retires, HP will be losing a great worker. I will miss him!

Deborah McLean:
Mike's enthusiasm will be greatly missed at the ASC MSRC. His undying dedication and work ethic should be an example for us all. Mike truly believed in the Outreach Program and its importance to the HPCMP. His love of people made him a natural as Outreach manager. Mike provided the ultimate example of an Outreach manager; it is now up to us to continue the effort.

Chuck Abruzzino:
What a guy to have as a friend and co-worker. He got more work out of me by just being...civil.

Jeff Graham:
I think Mike's next job could easily involve stand-up comedy. My fondest memory of Mike was his Outreach speech at the User's Group Conference in Houston back in 1998. Although the weather was a scorcher, Mike had the entire assembly cutting up as he discussed everything from cancer in mice to ships with mice. Following a keynote speech from Admiral Gaffney of the Navy, Mike used just the right mixture of goofy juxtapositions and malapropism to keep everyone in stitches for at least 15 minutes. Everybody in the program knew who Mike Moore was - and that ASC had a strong presence and commitment to Outreach. At first I didn't think he really knew what he was doing - but I certainly learned otherwise over the months and years that followed. Thanks for everything Mike - it was a fun ride!

Michelle Corcoran:
Count on him to do whatever it took. For over a year he handled the entire Outreach function himself. As a modest man, he would say a lot didn't get done. As a supervisor I always thought he did twice what I might have accomplished in the same position. He would say nothing grew during that time. But during that time, he laid a solid foundation for the future of Outreach after his retirement. He educated us all on what it took to do the job right and I believe that period was the beginning of great things.

years of service and dedication.

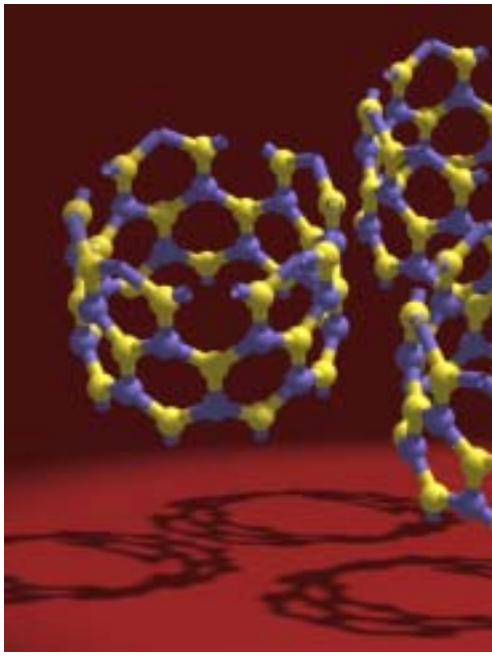
Hank Laughlin:
If you wanted to meet someone at a conference or show, then you went to Mike for an introduction. Mike knows everyone and everyone knows Mike.

Paul Shahady:
Mike is truly a "one of a kind"! His commitment to the DoD's High Performance Computing Modernization Program was demonstrated every day. He brought an enthusiasm to the HPCMP Outreach effort that will be hard to match. At the ASC MSRC, at the HPCMP, or at Supercomputing he will always win the "Mr. Congeniality" award. Good luck, Mike, on your new career.

Ruth Pachter:
I have worked with you since 1996 on many different projects. You have always been most helpful, even with last minute changes, professional and knowledgeable, always cheerful and in good spirits, at tours of the MSRC to visitors ranging from Dayton community leaders to congressional staffers, to ASC's commander and other dignitaries; in helping organize the User Groups meetings, the DoD booth at SC conferences, and booths at local conferences and meetings; and in endless other responsibilities, such as with the ASC MSRC Journal, or Outreach activities to users locally and at conferences--in short, if there was any quick action problem, or Outreach activity to be carried out, you were always happy and willing to help.

Jann Ensweiler :
In March of 1997, I came over to the ASC MSRC as the Human Resource representative. Mike was working on the ribbon cutting ceremony all by himself and so I asked Mr. Shahady if I could help Mike. Mike taught me so much about the technical aspect of the program and about Outreach. I would not be where I am today, as the Outreach Project Officer for the High Performance Computing Modernization Program Office, if it were not for Mike Moore.

A Comparative Theoretical Study of Carbon and Boron-Nitride Single-wall Nanotubes



From the time of their discovery, carbon (C)[1] and boron-nitride (BN)[2] nanotubes (NT) have been receiving ever-increasing interest due to their novel properties and potential application in nano-devices. Carbon nanotubes (CNTs), for example, can be either metallic or semiconducting depending on their chiralities and diameters[3], and these and other unprecedented properties suggest a variety of applications, as previously summarized[4]. However, applications are still hampered by the diversity of tube diameters and chiralities, and particularly aggregation in CNT samples obtained from various preparation methods, thus leading to studies on their separation and characterization, recently reported by Smalley's group[5], and also rendering theoretical predictions important. Calculations of structure and properties are also important for gaining insight into parameters that affect CNTs behavior, e.g., for field emission applications[6].

Raman spectroscopy has become promising in characterizing NTs, thus enabling the study of their optical and electronic properties. Previous work has shown a relationship between the Raman resonance energy and tube diameter[7], depending also on the excitation laser energy[8]. In our comprehensive theoretical study of CNTs and BN-NTs using all-electron and planewave pseudopotential (PW-PP) first-principle methods[6], we calculated the radial breathing modes (RBM), which are characteristic of NTs and do not have any corresponding modes in graphite, optimizing the geometry and cell parameters in all calculations. In tube bundles, we also obtained the equilibrium inter-tube distance.

We find[6] that the RBM values depend on the inter-tube separations in tube bundles, and are important to optimize[6] them for both CNTs and BN-NTs. The RBM values were fitted to A/R (shown in Figure 1), where R is the tube radius and A the fitting constant. Interestingly, our results agree well with recent experimental estimations of the RBMs in single-wall carbon NTs[9], and previous PW-PP calculations by Kurti et al.[10] The BN-NTs RBMs show a similar behavior as the CNT values. The fitting parameters (summarized in Table 1) in CNTs are larger than those in BN-NTs by about 8% and 10% for zigzag and armchair tubes, respectively. The van der Waals interactions alter the RBM values in tube bundles, and in order to understand the origin of this previously studied up-shift, the electronic structures were studied[6], such as the opening of a pseudo-gap due to the broken symmetry in metallic C (10,10) tubes.

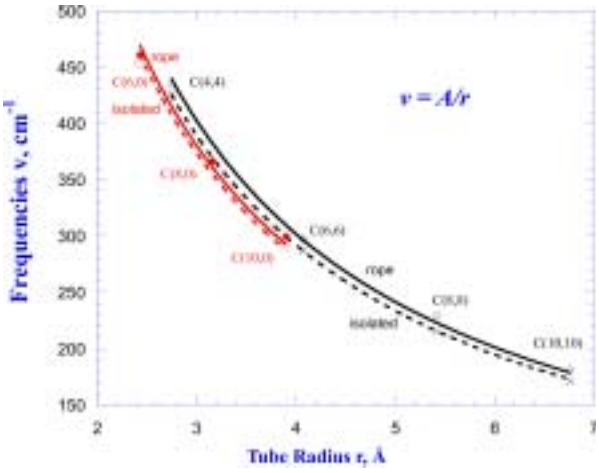
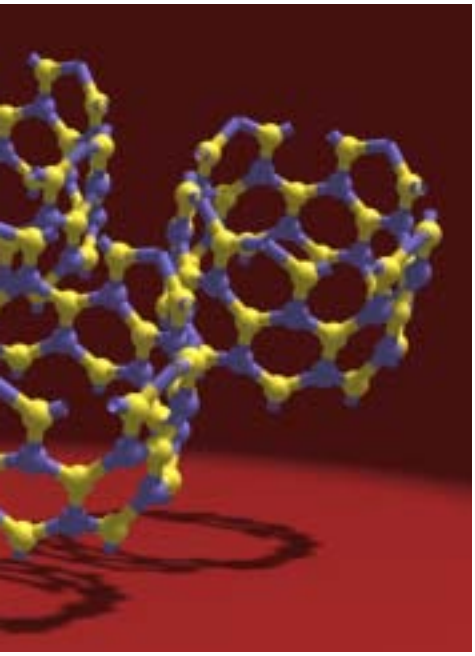


Figure 1. Calculated RBM vs. tube radius.

Table 1. RBM fitted (A [Å cm^{-1}]) to 1/R.

We would like to acknowledge AFRL support and the Major Shared Resource Center at ASC/HP.

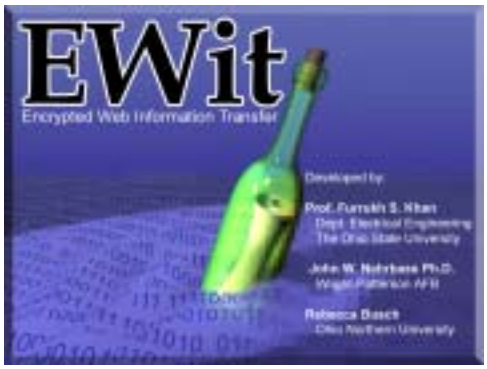


Researchers:
Xiaofeng Duan, ASC MSRC
Brahim Akdim, AFRL/MLPJ
W. W. Adams, Rice University, Center for Nanoscale Science and Technology
Ruth Pachter, ASC MSRC and AFRL/MLPJ

References
[1] S. Iijima, Nature (London) 56, 345 (1991).
[2] N.C. Chopra, R. J. Luyken, K. Cherrey, V. H. Crespi, M. L. Cohen, S. G. Louie, and A. Zettel, Science 269, 966 (1995).
[3] M. S. Dresselhaus, G. Dresselhaus, and Ph. Avouris, Eds., Carbon Nanotubes: Synthesis, Structure, Properties, and Applications, Vol. 80 (Spring, Berlin, 2001).
[4] R. H. Baugham, A. A. Zakhidov, and W. A. de Heer, Science 297, 787 (2002).
[5] M. J. O'Connell, S. M. Bachilo, C. B. Huffman, V. C. Moore, M. S. Strano, E. H. Haroz, K. L. Rialon, P. J. Boul, W. H. Noon, C. Kittrell, J. Ma, R. H. Hauge, R. B. Weisman, and R. E. Smalley, Science 297, 593 (2002).
[6] B. Akdim, X. Duan, W. W. Adams, and R. Pachter, Phys. Rev. Lett., to be submitted.
[7] J.-C. Charlier and Ph. Limbin, Phys. Rev. B 57 15037 (1998).
[8] P. Corio and M. Shapro, Phys. Rev. Lett. 86, 131 (2001).
[9] M. Strano and R. Hague, et al., personal communication.
[10] J. Kurti, G. Kresse, and H. Kuzmany, Phys. Rev. B, V 58, R8869, (1998).

Encrypted Web Information Transfer

by Chuck Abruzzino



The summer intern program gives the ASC MSRC an opportunity to tap into some of the brightest minds from universities across the country. The goal of this program is to challenge students with projects beyond their usual college classes. Now in its fifth year, this program provides the interns with real-world work experience and the mentors the opportunity to increase their involvement on the many projects supported by the PET program. One project in particular highlights how the entire PET and DoD community benefits from this program.

Mentor Dr. John Nehrbass, the on-site lead for Signal Image Processing, assigned summer intern Rebecca Busch, the task of redesigning a user interface for a much needed software system. (*See related article page 10*.) This system will potentially enable users to exchange large electronic data sets securely using existing high-speed connections. While Busch had extensive experience working with Java code, she had no previous experience with cryptography software. Provided with a rough working prototype of Encrypted Web Information Transfer (EWit) program, Busch quickly researched the functionality of the numerous lines of code and icons. She then methodically developed new dialogue boxes and graphics that help the user navigate through the complex procedures to prepare files for transfer. Members of The Ohio State University staff, along with her mentor, received her efforts with positive acclaim.

EWit was initially developed through the Department of Electrical Engineering at The Ohio State University and tested by the Electromagnetic Code Consortium (EMCC) community. Led by Professor Furrukh S. Kahn the project strives to build a self-contained, strong cryptographic software system, with full verification and authentication capabilities, that will allow the protection and secure distribution of sensitive unclassified electronic data. This system will enable transfer of secure data over unsecure channels such as the Internet. One of its unique features is that it will encrypt files as large as two gigabytes.

Consisting of two software components, the EWit client is a stand alone, self-contained application implemented in Java version 1.2. This is the cryptographic engine of EWit with implementations of strong cryptography features like symmetric and asymmetric ciphers, private key pass phrase protection, etc. Authentication and verification features include digital signatures, digests, and certificates. The system will use royalty-free algorithms widely available in the public domain.

The *EWit Server* is a web-based environment used for public key registration, public key distribution, automatic secure registration, and subsequent secure modification of user information. *EWit server* will also be implemented in Java 1.2 and will use Java servlets and Java server pages for server side processing. The users use the EWit client application to interface with the *EWit server.*

Since both the server and the client will be implemented in Java, the compiled code will be portable across various platforms and operating systems. Upon completion, the system will be hosted on a SUN server at the ASC MSRC.

As a result of the summer intern program and the EMCC community, EWit will soon be given version 1.0 status and made available to the DoD community.

The following algorithms are used in the EWit system:

Asymmetric Cipher:
Public Key Exchange: Deffie-Hellman

Symmetric Cipher:
Triple DES (DESede)

Symmetric Cipher for pass protecting private keys:
PBEWithMD5AndDES (64 bit salt, 20 iterations)

Hash Algorithm:
SHA-l

Signature Key Pair Algorithm:
DSA, 1024 bit keys

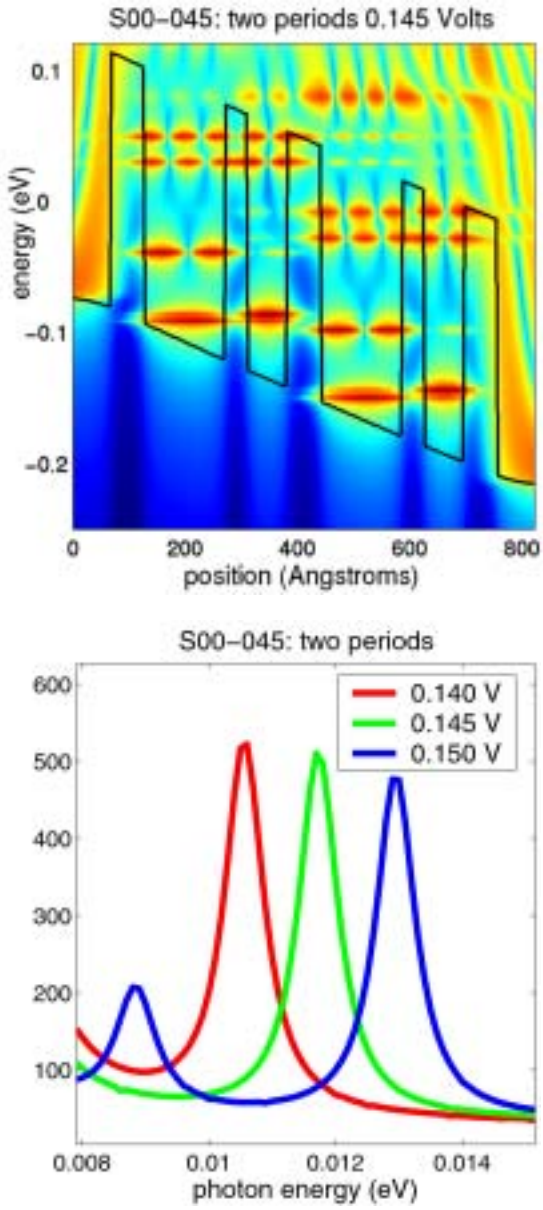
Exploring TeraHertz Laser Design Through HPC

by Dr. Paul Sotirelis

DoD researchers are collaborating with university partners to investigate the design of practical TeraHertz (THz) lasers. According to Thomas Nelson, Jr. (AFRL/SNDD), the principle investigator of an allocated HPCMP FY2002 project, "The design of a practical THz laser is a highly relevant research topic due to its potential for anti-terrorism use, such as the sensing of dangerous biological agents." It turns out that non-polar dry substances like paper, cardboard, plastic, thin pieces of wood, drywall, and ceramics are largely transparent to radiation in this spectral range. Furthermore, the THz spectral range is considered to be particularly important for identifying small yet complex cell-based microorganisms such as bacteria even at the strain level. Therefore, THz radiation is ideally suited for the remote nondestructive detection of dangerous biological agents, especially inside sealed packages, through the agent's own spectral signature. In addition to spectroscopic information, the use of THz radiation for three-dimensional imaging is currently undergoing intense research activity. Other military applications include its use for mine-threat detection, near space battlefield communication, and exo-atmospheric imaging radar.

Among the university collaborators is Professor L. Ramdas Ram-Mohan of Worchester Polytechnic Institute. According to Professor Ram-Mohan, "Practical means the laser must be small, portable, robust, efficient, intense, and somewhat tunable. This rules out methods more ideally suited for the laboratory." The most promising approach to fulfill these requirements is based on the quantum cascade laser (QCL) concept. QCLs result from sophisticated quantum engineering and semiconductor crystal growth of potentially thousands of layers. What makes QCL operation unique is that photons, which are emitted as electrons, cascade down the conduction band from one stage to another in an almost staircase like arrangement.

The first successful demonstration of a QCL was reported in 1994 by researchers at Bell Labs with emission in the mid-infrared frequency band. Recent research activity has been aimed at pushing operation into the far-infrared and THz frequency bands.



In the top figure, we show the self-consistent electronic density of states. The bottom figure shows the absorption coefficient for three different voltages. The structure used corresponds to one of two QCL designs denoted by S00-045.

The use of high performance computing is currently being explored to assist with QCL design. Jacob Gagnon, a Massachusetts Institute of Technology (MIT) undergraduate, worked on several algorithms during the summer of 2002 as a PET intern at the ASC MSRC. (*See related article page 10*.) It is hoped that Gagnon's work will allow the use of high performance computing to intelligently extract the best device structure from a statistical sample of devices. Personnel at the ASC MSRC are confident high performance computing will be helpful because our cost functions are based on the laser's essential physics. Gagnon will continue this work when returning to MIT this fall. Other collaborators include V. Menon (Princeton) and W. Goodhue (University of Massachusetts), and Paul Sotirelis (HPTi).

Specific Conductivity of Dilithium Phthalocyanine (Li_2Pc)

Two electrode impedance measurements were made on a thin film of dilithium phthalocyanine that was deposited onto a carbon substrate. The measurements were made from -50°C to + 100°C. The cell configuration used in the variable temperature experiment was: stainless steel electrode/thin film Li_2Pc cast onto carbon/thin film carbon on copper/stainless steel electrode. The total cell impedance varied from 3.4 to 4.6 Ω over this temperature range. The small change in resistance as a function of temperature suggests that a low energy of activation pathway for lithium ion transport has been achieved in the solid-state lithium ion conductor Li_2Pc. Specific conductivities are on the order of mS/cm over this temperature range.

Metal phthalocyanines can function as organic semiconductors because of overlap of the π molecular orbitals between adjacent molecules. The molecular system in our investigation, Li_2Pc, is used to form a lithium ion conducting channel via molecular self-assembly. A schematic of a one dimensional single ion conductor for lithium ions as shown in Figure 1 illustrates this point. The macrocyclic ring in this figure is an unsaturated macrocyclic complex such as dilithium phthalocyanine. It is by design that one uses an unsaturated macrocyclic complex because with it, there is electron delocalization around the ring that keeps the lithium ion centered within the macrocycle. Correspondingly, this is where the negative electrostatic potential is at a maximum. It is through proper spacing of the unsaturated macrocyclic rings, with respect to one another, that allows one to create a channel where the negative electrostatic potential remains relatively constant throughout the molecular system but where there is sufficient macrocyclic ring separation to preclude electronic conduction. It is the relatively constant negative electrostatic potential that is primarily responsible for changing the lithium ion transport mechanism from one that depends primarily on polymer segmental motion as found in oxygen based polymer electrolytes, to one that depends upon the electric field gradient established between the electrodes of a cell. In this fashion, the temperature dependence for ionic conduction is minimized and one can expect high ionic conductivity at ambient and subambient temperatures.

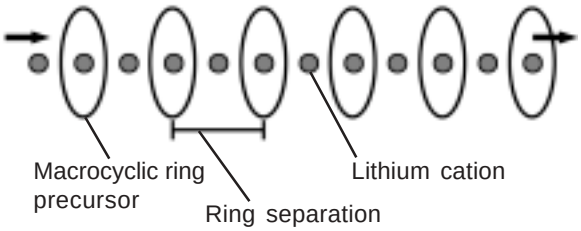


Figure 1. Schematic diagram for a one-dimensional single-ion conductor for lithium ions.

In order to test the concept of a lithium ion conducting channel based on Li_2Pc, the molecular structures for Li_2Pc and $(Li_2Pc)_2$ were optimized using Density Functional Theory. These calculations were performed at the ASC MSRC using the Gaussian 98 computational chemistry program and the B3LYP hybrid functional.

Figures 2 and 3 show the calculated structures using the 6-31G(d) basis set. The separation between lithium ions in Li_2Pc is 1.991 Å. Lithium nitrogen bond distances are 2.18 Å. The calculated electronic energy for Li_2Pc at 0 K is – 1682.3574567 Hartrees. $(Li_2Pc)_2$ as shown in Figure 3 represents the molecular structure after two adjacent molecules of Li_2Pc have combined through electrostatic forces. The calculated electronic energy for $(Li_2Pc)_2$ at 0 K is -3364.743437 Hartrees. The calculated bond energy between the two phthalocyanines as a result of the electrostatic attraction is 17.90 kcal/mole. The separation between lithiums that are almost in the plane of the phthalocyanine rings is 4.47 Å. The phthalocyanine rings are staggered now

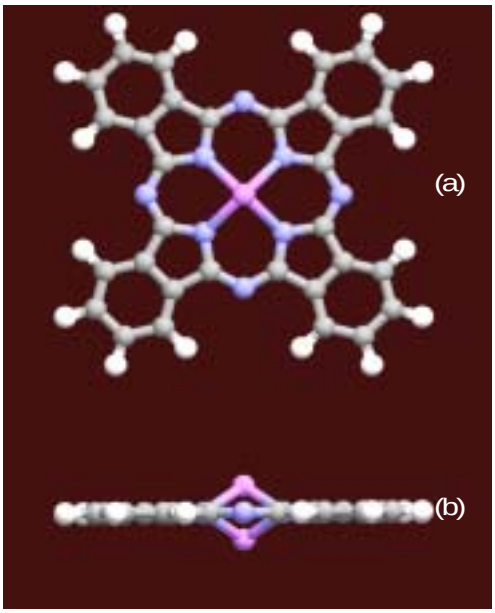


Figure 2. Optimized geometry for (Li_2Pc) (a) top and (b) side views using the 6-31G(d) basis set for optimization.

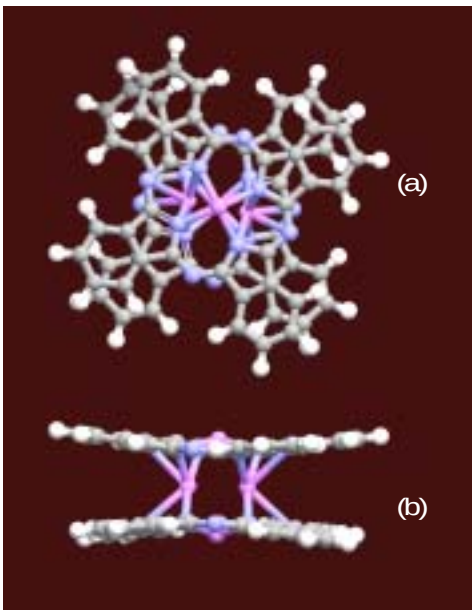


Figure 3. Optimized geometry for $(Li_2Pc)_2$ (a) top and (b) side views using the 6-31G(d) basis set for optimization.

by approximately thirty degrees. The separation between the outer benzene rings varies from 3.94 to 4.89 Å. These values were measured between the two carbons that overlap one another on the outer benzene rings. The importance of these calculated results suggest that molecular self-assembly can be important in the formation of the lithium ion conducting channel and one might expect high electronic resistance due to poor orbital overlap between the π molecular orbitals.

Researchers:
L. G. Scanlon
Air Force Research Laboratory, Energy Storage and Thermal Sciences Branch, WPAFB
L. R. Lucente
University of Dayton Research Institute
W. A. Feld
Department of Chemistry, Wright State University
G. Sandi
Chemistry Division, Argonne National Laboratory
R.E. Gerald
Chemical Technology Division, Argonne National Laboratory
R. Klingler
Chemical Technology Division, Argonne National Laboratory
R. Csencsits
Materials Science Division, Argonne National Laboratory
S. J. Rodrigues
University of Dayton Research Institute

Fieldview Vendor Day

by Darwin Adams

As a part of the ASC MSRC Scientific Visualization (SciVis) Laboratory Advocacy Program, a recent Vendor Day event featured software available to the Computational Fluid Dynamics (CFD) user. This program was developed to promote the overall offerings available within the SciVis Laboratory. Participants are introduced to software, hardware, and support services available within the Laboratory and the ASC MSRC. In addition to Vendor Days, which focuses on a single vendor's software package, Technology Days and SciVis Open House Days are also offered. Technology Days showcase updates and the latest developments of software packages with an emphasis on researchers from specific CTAs. SciVis Open House Days focus on researchers wanting a more general introduction to the technologies and capabilities available within the Laboratory.

Fieldview 8 was featured during the third Vendor Day event on August 12. A group consisting of half-dozen researchers attended the event in two sessions. The morning session was constructed to allow time for a facility tour and a SciVis demonstration of the ImmersaDesk, a virtual model display system. The afternoon session was targeted to researchers familiar to the ASC MSRC SciVis facility that did not require the facility tour or SciVis demonstration. Both sessions brought together users from the Air Force Research Laboratory's Propulsion and Air Vehicles Directorates to meet with representatives from Intelligent Light, makers of Fieldview. The event provided the opportunity for CFD users to determine how Fieldview Version 8.1 and its stereo capability may assist in research efforts.

The open format of this event allowed the technical exchange to be directed to current problems encountered by the attendees. The targeted presentation was considered worthwhile among all participants. Through these events, the ASC MSRC SciVis Laboratory has empowered both research and software communities to focus on identifying pre- and post-processing and visualization solutions to better enable research activities. (*See related article page 4*.) The researcher has an opportunity to address concerns and resolve complex visualization problems. The software vendor has an opportunity to instruct and inform attendees of software enhancements, techniques, and new products.

Additional events will be scheduled throughout the remainder of the year. A request for information should be emailed to *msrcenws@asc.hpc.mil*.

SGI Origin 2000 Relocated

by Nicholas Voiles

Electronic excitement was in the air as Major Jim Forsythe of the United States Air Force Academy (USAFA) stopped by to pick up the SGI Origin 2000 from the ASC MSRC computer floor. Major Forsythe, the HPC point of contact for the academy, stated that they had a 64-processor high performance computer now, but were eager to take advantage of the HPCMO's program of re-locating high performance computers to the different service academies following MSRC updates.

The relocation of the Origin 2000 began when Major Scott Morton, the Director of the Modeling and Simulation Research Center at the USAFA, submitted a proposal to obtain a more advanced supercomputer. By acquiring a supercomputer, the USAFA hoped to accomplish the following:

1) Place increased emphasis on Air Force high performance computing to boost declining Air Force participation.

2) Facilitate expanded modeling and simulation research across all USAFA science and engineering facilities and research.

3) Enrich cadet experience, improving support of AFRL and other Air Force and DoD organizations in their missions.

Major Forsythe rented a truck to transport the 128 processors back to the Air Force Academy in Colorado. These processors will help the USAFA to achieve their goal of creating an environment that allows faculty and cadets to perform cutting-edge modeling and simulation research in support of Air Force research programs.

The DoD Institutions of Higher Learning Program has once again proven very effective. The goal has been met to provide HPC opportunities to DoD service academies and institutions of higher learning in order to prepare our future military leaders to excel in tomorrow's technologically complex world. Major Forsythe and Major Morton are to be congratulated for their efforts to upgrade the USAFA's computer center, and giving the students of today the opportunity to excel as leaders tomorrow.

Information Environment Update

by Nicholas Voiles

Over the past year, work has continued on the DoD HPCMP's web based Information Environment (IE) initiative. Charlotte Coleman first brought this project to our attention in the Spring 2001 issue of the ASC MSRC Journal. The vision and goal of this initiative have remained unchanged since its inception. The vision is to create a program-wide information infrastructure that benefits both the user community and resource center support staff. The goal is to provide the HPCMP community seamless access to distributed relational data, improve information sharing/gathering about HPCMP associated sites, standardize data exchange/reporting, and integrate data into a common information architecture.

Phase one of the IE initiative will provide common user interface to five specific capabilities, oriented towards three end-user communities. The first community is the scientist/researcher, secondly the S/AAAs, and finally the HPCMP community. A team from the ASC MSRC has recently completed phase one. Phase two is being worked out through an IE Integrated Product Team (IPT), working with the HPCMO on vital enhancements and other modifications to improve the functionality. At this point in time, Ms. Valerie Thomas of the HPCMO has taken over the program management for phase two, assisted by the IE IPT.

IE has been undergoing developmental testing since May and has been accessible to MSRC users as a test system on the web. According to Jeff Graham, IE host site manager at the ASC MSRC, "The IE schedule has been revised recently as the managers and IPT have been working hard to get it up and running by November of this year. The users and managers of the program are all excited about the potential in cutting back their paper-oriented workload."

Future capabilities will allow those in the scientist/researcher community to query process status, which will display the status of jobs submitted to any system within the program, via the web. User fill-in will also be included and via the web, users will be able to update their own user/project information.

The S/AAA community will have access to allocation management, which will allow an S/AAA via the web to move hours amongst their own projects or swap hours with another S/AAA of the same service or between services. Account application management will provide S/AAAs with web-based capability, to generate required paperwork for opening accounts, managing/tracking and processing allocation requests.

In the HPCMP community, allocation/utilization reporting will be included and will provide users, site staff, S/AAAs, and HPCMO access, via the web, to utilization and allocation information.

The IE system will be available to those users from the four MSRCs and various Distributed Centers. ASC will serve as the host site for the IE initiative. Even though it is the host site, ASC will also be a non-host site. Along with the HPCMO, the other non-host sites are:

- Army High Performance Computing Research Center (AHPCRC), South Minneapolis, Minnesota;
- Army Research Laboratory (ARL), Aberdeen Proving Ground, Maryland;
- Arctic Region Supercomputing Center (ARSC), Fairbanks, Alaska;
- Army Engineer Research and Development Center (ERDC), Vicksburg, Mississippi;
- Maui High Performance Computing Center (MHPCC), Kihei, Hawaii;
- Naval Oceanographic Office (NAVO), Stennis Space Center, Mississippi;
- Naval Research Laboratory (NRL), Washington, DC;
- Space and Missile Defense Command (SMDC), Huntsville, Alabama.

When fully operational, IE will offer a secure web-based information environment, which will benefit many users throughout the country. Important steps remain, but the system will soon be ready for use. For more info and the latest updates contact *asc.hp.outreach@wpafb.af.mil.*

Outreach

Reaching Out

by Nicholas Voiles

The ASC MSRC Outreach Team began their spring conference tour in sunny San Diego, California at the annual Advanced Simulation Technologies Conference (ASTC), April 14-18. As in the past, business cards were turned into luggage tags for a popular giveaway. The MSRC's booth was the hit of the show as they were paired up with the team from the Simulation and Analysis Facility (SIMAF), who brought their hardware and software, which together simulate an F-16 with modified Joint Strike Fighter (JSF) capabilities. One of the highlights from the conference was the keynote speaker Ms. Jacqueline Steele from the U.S. Army Space and Missile Defense Command (SMDC), who discussed Modeling and Simulation Economics. Her discussion presented cost effective tools that impact testing processes and offer opportunities to do things cheaper and faster.

Next in line was the 3rd annual National Aerospace Systems and Technology Conference (NASTC) held May 14-15. This Dayton-based conference focused on the technologies and resources needed to deliver war-winning capabilities. Approximately 800 research and acquisition professionals representing the Air Force, industry and academia, attended this conference. Once again SIMAF shared the MSRC booth, and many visitors learned to fly using high tech simulation hardware and software. Visitors to the booth included ASC Commander Lt Gen Richard V. Reynolds, AFRL Commander Maj Gen Paul Nielsen, and the Director of Aeronautical Enterprise Program Office Brig Gen Rosanne Bailey.

Dayton, Ohio was once again the site for the Greater Dayton IT Alliance ITEC technology event. This conference took place June 26-27, and featured many exciting speakers and exhibitors. For this show, the MSRC shared a large booth with SIMAF and the Chief Information Officer (CIO), both branches of the Information Technology (IT) Directorate. SIMAF was there again with their flight simulators and the CIO demonstrated their web-based knowledge tools Livelink and Facilitate.com. This collaboration between the three departments within the IT Directorate worked well and added variety to the booth. Many visitors were lured in by the MSRC demonstrations and SIMAF simulators, and in turn got to learn a little about the whole IT Directorate. Each section of the booth added to the excitement of the conference and attracted many potential customers.

If you would like to learn more about the ASC MSRC presence at these conferences or are interested in other Outreach activities, please contact us via email at *asc.hp.outreach@wpafb.af.mil*.

A Look Back

by Mike Moore

As I near retirement, I look back over my years at the MSRC with many fond memories.

When I joined the Program in 1994 the ASC was a shared resource center with an Intel Paragon high performance computer. My first "real" outreach task was stuffing envelopes with a newsletter containing helpful programming hints for our users.

In 1995, I began working on the Defense Research Engineering Network at the Program Office. In D.C., I was able to see the "big picture" as it related to high performance computing. While there, I was tasked with developing a video and posters for SC95, publicizing the computer center run by the 88th Comm Group. While attending SC95, I met Lynn Parnell, who was responsible for the HPCMP presence at SC95. Lynn provided me a brief glimpse into all that goes on behind the scenes of these conferences.

During those early years of the program, I worked as much for the Program Office as I did for the ASC MSRC. Much of the years 1995-1997 remains a blur in my mind. One thing remains crystal clear, at least in my little world. Hank Laughlin, Cynthia Payne, Jann Ensweiler, Program Director Paul Shahady, and Deputy Program Director John Blair were inseparable at work. Locally Cynthia, Jann, and I were the Outreach team; Cynthia was Mr. Shahady's secretary, Jann was the personnel officer, and I was a computer scientist. In those first months we were just a small group of employees working toward a common goal.

The ASC was named a Major Shared Resource Center (MSRC) in 1996. On-site personnel led by Jeff Graham and the Programming Environment and Training (PET) staff were asked to organize the 7th annual DoD User's Group Conference (UGC). The conference was held in the Beckman Building on the campus of the University of Illinois, Champaign-Urbana. I had the pleasure of meeting Larry Smarr of the National Center for Supercomputing Applications (NCSA), a man who briefed presidents on the future of technology. Dr. Anita Jones, HPCMO Program Director spoke to the conference attendees via Multicast. It seemed a little jerky and the bandwidth was certainly not very much, but we were all impressed.

In 1997 the Naval Oceanographic Office (NAVO) MSRC and its integrator Northrup Grumman sponsored UGC in La Jolla, California. Attendees were able to take high performance computing tutorials on computers set up in the Marriott. I remember Nahid Sidki of the HPCMO being all over the hotel getting computers to work for the tutorials.

The U. S. Army Corps of Engineers Waterways Experiment Station (now ERDC) MSRC and the Shared Resource Centers Advisory Panel (SRCAP) sponsored the UGC held at Rice University in 1998. I made my speaking debut in Houston when Steve Schneller of SRCAP allowed me a few moments to speak to the group about SC98.

The lone cypress, Pebble Beach and cool temperatures of Monterrey, California greeted the 1999 attendees. Judith Bouchelle-Keithly spearheaded the effort for the Army Research Laboratory (ARL). In her keynote address, Delores Etter, Deputy Undersecretary of Defense (ST), spoke of the partnerships within the DoD. She stated that there are a lot of players in the DoD that can benefit from the HPCMP. In 1999, the ASC MSRC did not own a telescopic lens for our camera. To get pictures with high enough resolution for print, I had to get within a few inches of a person's face; even if the person was speaking in front of 300 people. Thus I became known as the camera man. Even though the MSRC now has cameras with telescopic lenses, the name remains.

By the year 2000 it was again ASC's turn to sponsor the UGC. Under the leadership of Jeff Graham and Maria Zimmer the ASC team did an exhaustive analysis to determine the host site. From a list of 20 cities the list was narrowed down to Albuquerque and Las Vegas. Jann Ensweiler, Susan Vega, and Steve Baxter then toured both cities and reported their findings to Cray Henry, HPCMP Director, who then chose Albuquerque. Prior to UGC 2000 Jann was splitting her time between the ASC MSRC and the Program Office. After UGC, she transferred to the Program Office in Arlington. While the Program Office gained an experienced Outreach campaigner, I lost a valued co-worker.

Keynote speaker Kay Howell gave attendees a look into the method the President uses to determine how to spend the science and technology money and how it is allocated. Dr. Robert Peterkin, Dr. Suresh Menon, and Dr. Edwin Rood each gave a user's perspective on high performance computing.

Along with SC98 and SC01, I feel that the 2000 DoD UGC was the ASC MSRC's finest hour. Sometimes when you work the hardest, you feel the most satisfied with the final product. Putting on a User's Group Conference requires an intense effort by the MSRC employees for a period of months, but the feedback gathered from the users makes it all worthwhile.

NAVO again served as the host for UGC in 2001, which was held in Biloxi, Mississippi. It was evident at this conference that the attendance had shifted from managers of the shared resource centers to users. Users were able to see various kinds of on-going projects. Papers presented highlighted the revolutionary changes that the HPC user has been able to accomplish the last couple of years.

Austin, Texas was the setting for the most recent UGC held in June 2002. Dave Stinson, Rose Dykas and the team from NAVO met the challenge of organizing this conference. Steve Scherr served as conference chair.

Keynote speaker Dr. Charles Holland, Deputy Under Secretary of Defense (DUSD) Science and Technology (S&T) spoke on the mission and the vision of DUSD S&T. Dr. Holland identified three transformation initiatives important to the DoD; the National Aerospace Initiative, the Advanced Surveillance and Knowledge Systems Initiative, and the Power and Energy Technologies.

Cray Henry presented the HPCMP Director's Report. Cray stated that at over 100 sites the HPCMO is serving 607 projects and 4,023 users. For FY03 the program has non-real-time requirements of 77.5 teraflops-years. According to Cray there are 1,103 users of CFD, 540 users of CSM, 33 users of CEN, and 200 users of EQM. In the modeling and simulation area, there are 306 SIP users, 650 IMT users, and 280 FMS users. Included in the briefing were Corporate Initiatives, which are problems or requirements needed by the HPC community and that are being solved by in-house project teams. IE (*See related article page 24*.), metacomputing, benchmarking, mass storage and archiving server are challenges being solved by HPCMP folks, not by outside vendors.

The User Group social was held at the Bob Bullock Texas State History Museum, named for the state's 38th lieutenant governor. In the IMAX theater, attendees took a virtual tour of the Space Lab's living quarters in "Space Shuttle". The museum tells the story of Texas through exhibits, theaters, films, and interactive computer displays. The museum lobby's design depicts figures from Texas history around a campfire, along with a 50-foot granite map of Texas.

Approximately 400 participants attended this year's conference. I remember when we could barely get 200 folks at the conference and all of them were center managers. We have succeeded in making this truly a user's conference, evident by the fact that approximately two thirds of the attendees were users.

UGC 2003 will be hosted by the HPCMO in Bellevue, Washington. The User Advisory Group leader Steve Finn will serve as chair.

As we have seen change through the years at the UGCs, so it is true for the Outreach group at the ASC MSRC. As of September, I will retire. While I will miss all my friends in the HPC community, I will be enjoying life in Madison, Indiana, where all of you all are welcome to visit.

To all of you who have assisted in various Outreach activities, a hearty thank you! Many of you went above and beyond to get the job done. My job was enjoyable because of you. Working together we were able to accomplish great things the last eight years. I leave feeling fortunate to have worked along side some of the very best.

While space will not allow me to recognize each person I have worked with individually, I must mention a

few. Larry Falb and Gary Louden spent a year working twelve-hour days at the Program Office. I only spent five months there and that was tough enough.

Two unsung heroes in my work-life are Margaret Smith and Sharon Brown. These two ladies are the first faces visitors see when they arrive at the ASC MSRC. They helped me immensely with many projects through the years.

My hat is off to the CSC Outreach team of Chuck Abruzzino, Joe Marler, and Deb McLean. Chuck deserves the credit for the ASC MSRC's outside image. I have seen Chuck make the most tedious technical article into a masterpiece of art. Thanks to Joe for helping me create two HP videos. Thanks to Deb for editing all the articles that I have written over the years. She raised the level of professionalism of the MSRC Outreach activities way above standard commercial efforts.

I must also mention the Outreach team that I worked with for the last year. Tonya Lankheit spent the last year, learning everything that I know about the philosophy of the HPCMP. She picked up on everything in thirty minutes and I spent the year watching her work. Thank you to Barb Little and Michelle Corcoran for recognizing potential when Tonya applied for the job.

Pat Montanaro was responsible for bringing Nicholas Voiles to the MSRC as a co-op student in the summer of 2001. A recent graduate of Wright State University, Nick has a degree in marketing. He knows the stuff about Outreach that took me years to learn.

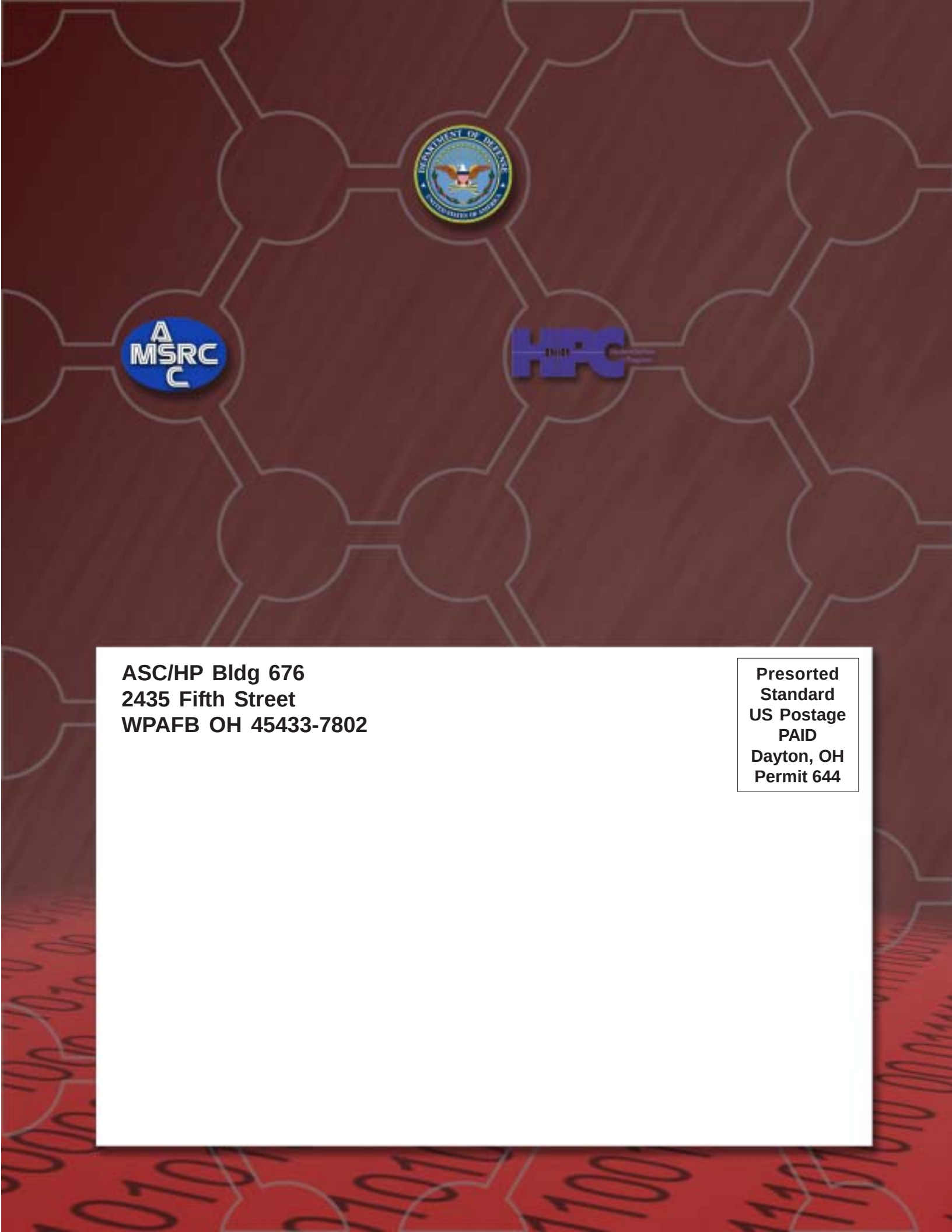
I know you will enjoy working with both Tonya and Nick. I am confident that I leave the Outreach tasks in very capable hands.

Finally I thank my last boss, Michelle Corcoran. With her touch, the Outreach Program became a more professional organization.

Thanks for the memories!

Point of Contact
ASC MSRC Customer Support
web site: http://www.asc.hpc.mil
email: asc.hp.outreach@wpafb.af.mil
Phone: 1-888-MSRC ASC
(1-888-677-2272)

ASC MSRC Journal *is published by the CSC Customer Assistance Center ASC MSRC WPAFB, Ohio. Your comments, ideas and contributions are welcome. Any opinions, findings, conclusions or recommendations expressed in this publication are those of the author(s) and do not necessarily reflect the views of the DoD. All photographs were taken by ASC MSRC staff, unless otherwise noted.*



ASC/HP Bldg 676
2435 Fifth Street
WPAFB OH 45433-7802

Presorted
Standard
US Postage
PAID
Dayton, OH
Permit 644